

"Instrumentation" for Theory Modeling and Simulation (TMS) in Nanoscience

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CNMS Lehman Review, July 21 2004

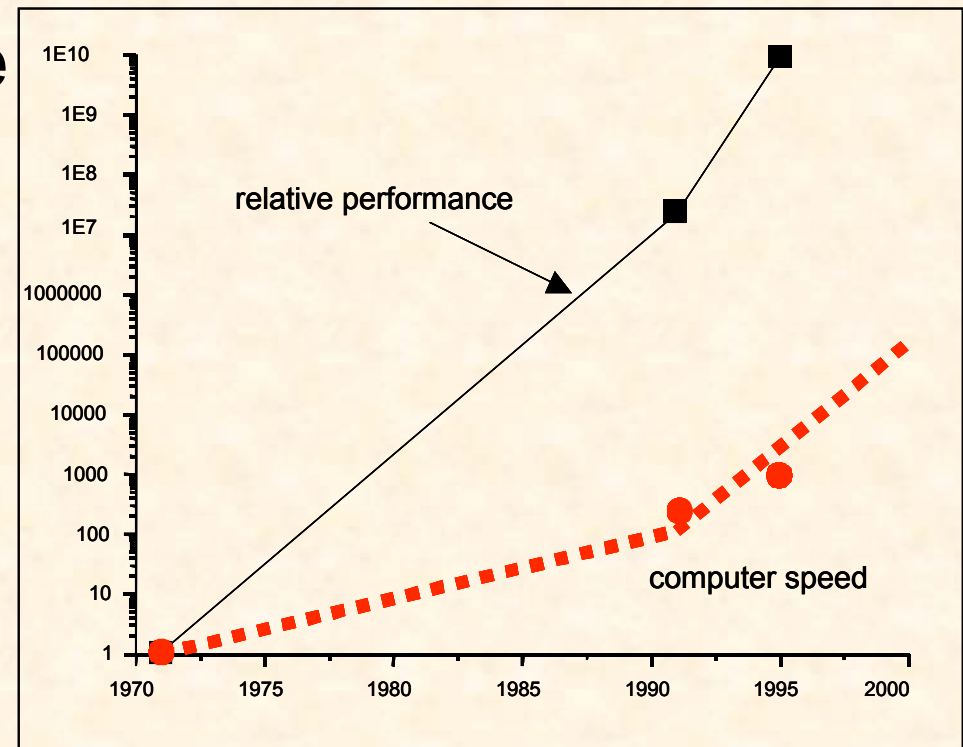
TMS in a user facility: the challenges

- **Diversity of scientific problems**
 - Need many specialists to cover all TMS needs
 - support experiments
 - develop TMS methods, algorithms, codes
- **Computers lifetime (3-5 Yrs) is short compared to TMS methods and codes (>20 Yrs)**
 - Keep rebuilding / reinventing the “wheel”
- **“Genius effect” that can make any center based effort look bad**

The reality of “big-science” on big computers and in user centers

(D. P. Landau, UGA)

- The goal is the science and the computer is a tool
- Very high payoff from improvement in algorithms / methods
- Most algorithmic / methodological improvements happen in “small shops”
- Need a scalable architecture / approach (!)



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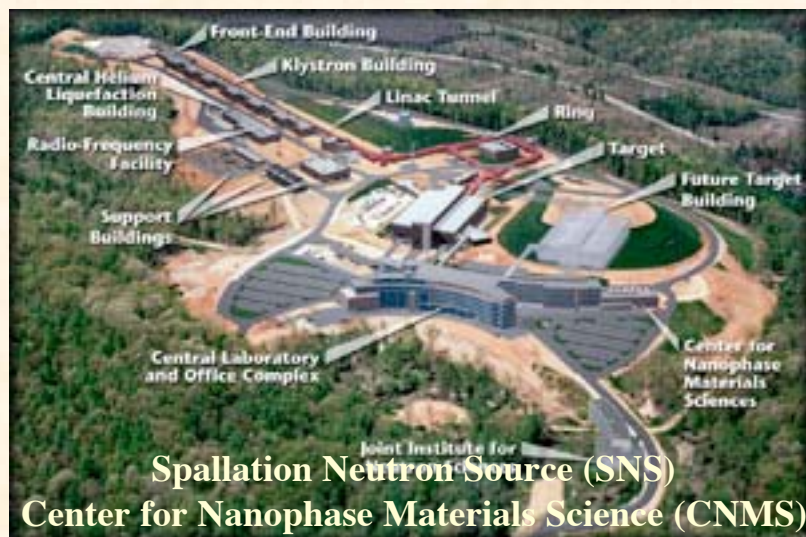
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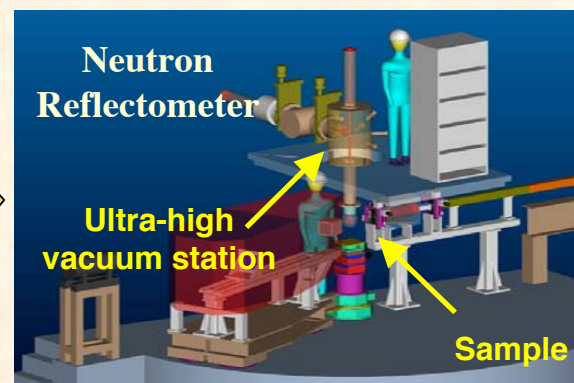
TMS in a user facility: how to meet the challenge

- **Engage the best in the community**
 - Leadership Scientific Computing Facility (LSCF)
 - Excellent experiments at CNMS
- **Be flexible with staffing**
 - Draw from ORNL staff and assign portions of FTEs depending on the needs of the CNMS
 - Postdoctoral fellows dedicated to CNMS
- **Run an extensive visitor program**
 - Long terms visitors (~1 year)
 - Nanoscience Focused User Laboratories (NanoFocUL) first series in Summer 2004
- **Coordinate CNMS/NTI activities with Center for Computational Sciences' Materials Research Institute**
 - Join forces in developing repository for nanoscience, condensed matter physics, and materials science

New Approach: Facilities analogy



Facility



Instrumentation



User
Community



**Materials Science
Virtual User Center**
**Materials : Math : Computer
Scientists**

- *Open Source Repository*
- *Object Oriented Tool Kit*
- *User Laboratories*
- *User training*

User
Community

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New world-class facility will be housing leadership class computers

- **Space and power:**
 - 40,000 ft² computer center with 36-in. raised floor, 18 ft. deck-to-deck
 - 8 MW of power (expandable) @ 5c/kWhr
- **Classroom and training areas for users**
- **High-ceiling area for visualization lab (Cave, Powerwall, Access Grid, etc.)**
- **Separate lab areas for computer science and network research**



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LSCF: Roadmap 2004 - 2008

High-End Science



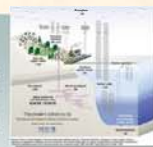
climate



fusion

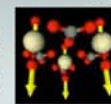
nanotube modeling

2D supernovas



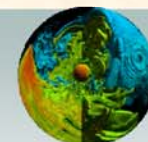
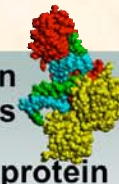
atmospheric chemistry

multi-scale modeling



protein machines

protein function



3D supernovae

People



Programs

SciDAC

GTL

Nano

FSP

Core programs in science, math, computer science, networking

Partnerships

Labs

Universities



World class facility & connectivity



ESnet

Internet 2

TeraGrid

NLR

Ultrahnet

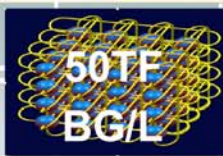
Sustainable path for Leadership Class computers



X1



X1e RS



50TF
BG/L



X2



100 TF
Sustained

2004

2006

2008

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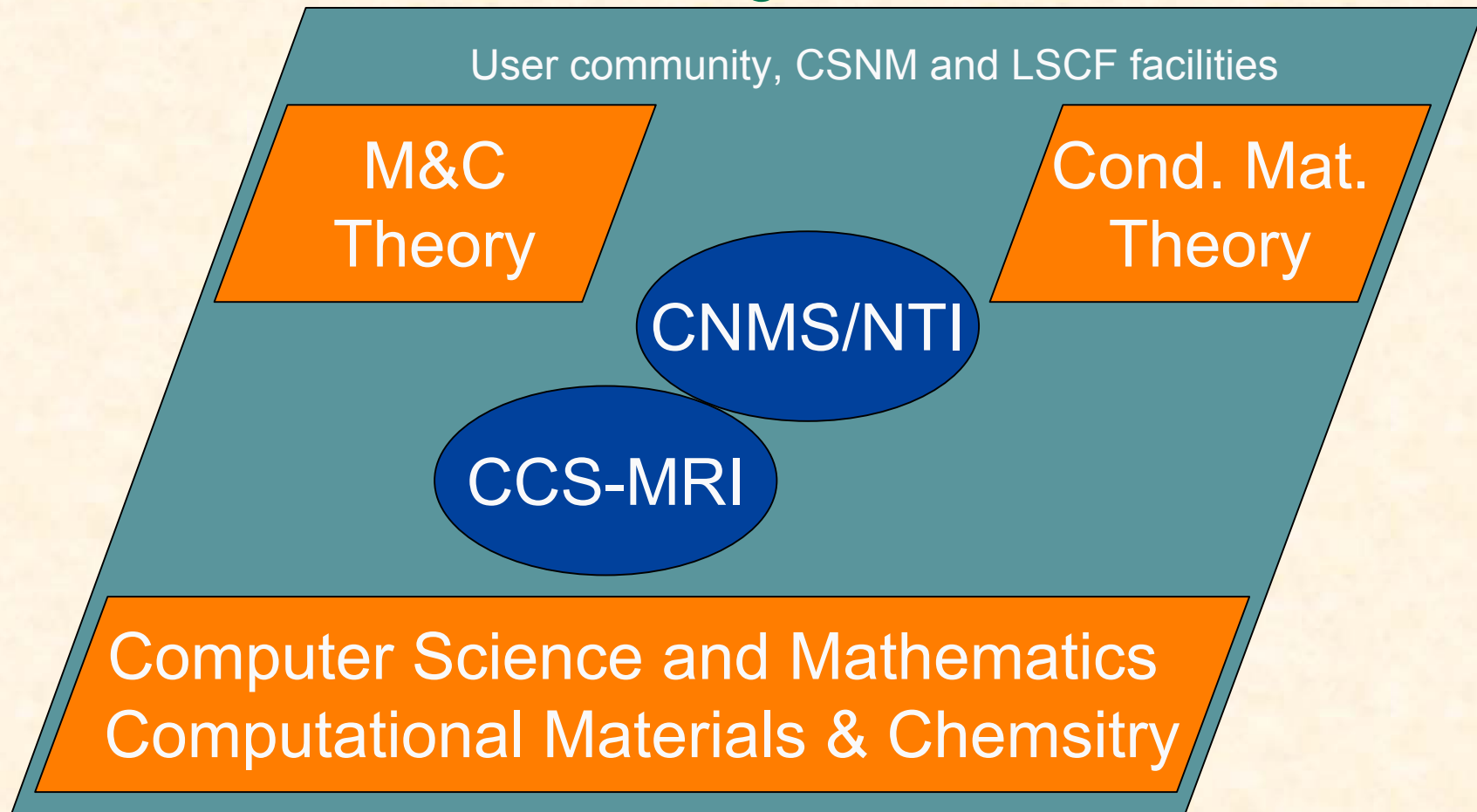
Common interest of CCS and CNMS

- **Deliver high profile science**
- **Maximize performance of applications on LSCF hardware**
 - **CCS: enormous challenge but materials science community has outstanding record**
 - **CNMS: maximize use of LSCF hardware for nanoscience**
- **Relevant to national nanoscience needs**
 - **CCS: nanoscience end-station was one of four high priority areas the LSCF is committed to build**
 - **CNMS: obvious**

CNMS/NTI and CCS-MRI coordination

- **Fundamental Research Enclave**
 - New network enclave for fundamental research
 - Simplify access to external users
 - Same security standard as ORNL's network
- **NanoFocULs run in JICS building on CCS computers**
- **Initiated development of repository**
 - NanoFocUL on nano-science end-station
 - Joint proposal in Tera-scale computing initiative
- **MOU for access to CCS' LSCF platforms is currently being worked out**

How ORNL's theory effort can benefit



- **Coordinate ORNL's theory effort**
- **Facilitates hiring of high quality new staff**

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UT-BATTELLE

TMS in a user facility: challenges and how we meet them

- **Diversity of scientific problems**
 - Many specialists needed to
 - support experiments
 - develop TMS methods, algorithms, codes
- **Computers lifetime (3-5 Yrs) is short compared to TMS methods and codes (>20 Yrs)**
 - Keep rebuilding / reinventing the “wheel”
- **Genius effect that can make any center based effort look bad**
 - Un-foreseeable algorithm & methods improvement can outdo any planned hardware investments
- **Join forces with CCS and it's LSCF**
 - Develop computational science instrumentation (end-station) for LSCF
- **Engage the best in the community**
 - Leadership Scientific Computing Facility (LSCF)
 - Excellent experiments at CNMS
- **Be flexible with staffing**
 - Draw from ORNL staff and assign portions of FTEs depending on the needs of the CNMS
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- **Run an extensive visitor program**
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Ongoing user projects

Three user projects and three CNMS Scholars

(note: theory was not part of original call for proposal)

- **Formation of hydrogel materials through formation of hydrophobically modified polyelectrolytes**
 - PI: Eric Luijten (U. Illinois), co-organizer of a NanoFocUL
 - CNMS Scholar: Lei Guo
- **Molecular- and Nano-wires: properties and control**
 - PI: Hai-Ping Cheng (U. Florida), co-organizer of a NanoFocUL
 - CNMS Scholar: Chun Zhang
- **Calculating time-dependent effects from a modified Wang-Landau density of states**
 - PI: Mark Novotny (Miss. State U.)
 - CNMS Scholar: Terrance Dubreus